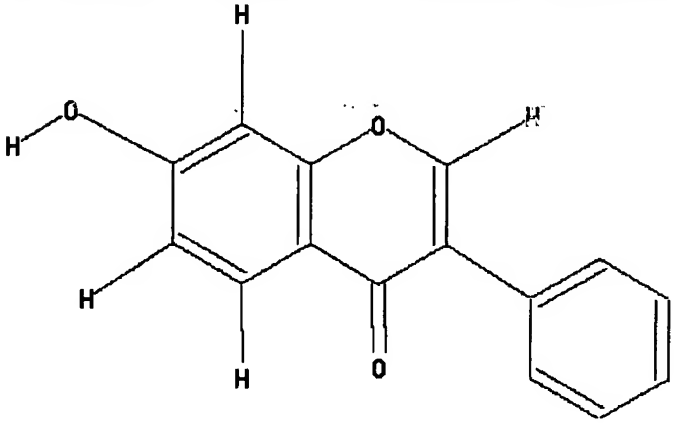
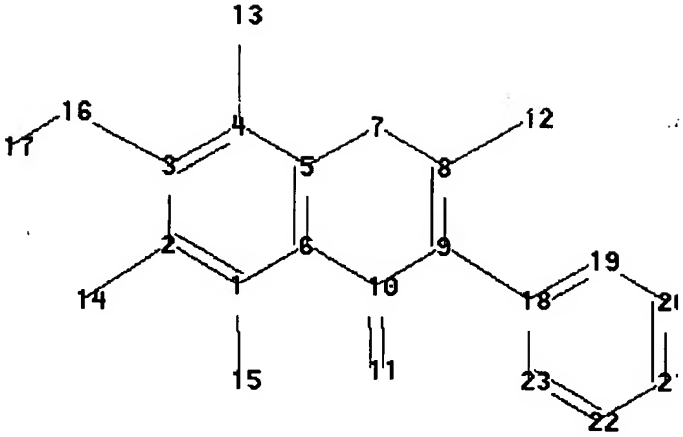
Connecting via Winsock to STN

FILE 'STNGUIDE' ENTERED AT 19:27:21 ON 20 OCT 2007

FILE 'REGISTRY' ENTERED AT 19:50:31 ON 20 OCT 2007

=>
Uploading C:\Program Files\Stnexp\Queries\10523964C.str



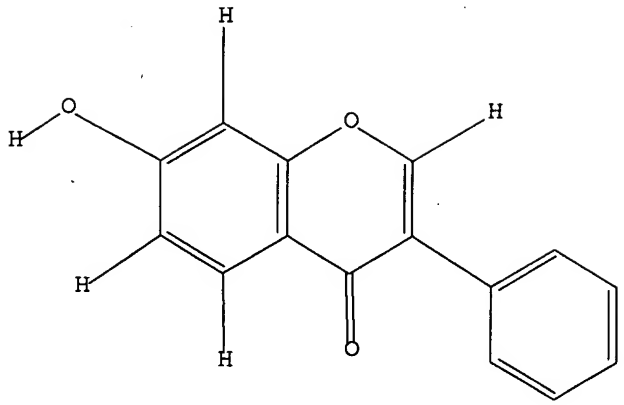


chain nodes :
11 12 13 14 15 16 17
ring nodes :
1 2 3 4 5 6 7 8 9 10 18 19 20 21 22 23
chain bonds :
1-15 2-14 3-16 4-13 8-12 9-18 10-11 16-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 18-19 18-23 19-20 20-21 21-22 22-23
exact/norm bonds :
3-16 5-7 6-10 7-8 8-9 9-10 10-11
exact bonds :
1-15 2-14 4-13 8-12 9-18 16-17
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 18-19 18-23 19-20 20-21 21-22 22-23

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:Atom
19:Atom 20:Atom 21:Atom 22:Atom 23:Atom

L5 STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s sss sam l5
SAMPLE SEARCH INITIATED 19:52:14 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1696 TO ITERATE

100.0% PROCESSED 1696 ITERATIONS 10 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 31450 TO 36390
PROJECTED ANSWERS: 11 TO 389

L6 10 SEA SSS SAM L5

=> s sss l5 full
FULL SEARCH INITIATED 19:52:33 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 33000 TO ITERATE

100.0% PROCESSED 33000 ITERATIONS 289 ANSWERS
SEARCH TIME: 00.00.01

L7 289 SEA SSS FUL L5

=> save l7 temp aver10523964/a
ANSWER SET L7 HAS BEEN SAVED AS 'AVER10523964/A'

=> fil caplus
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	174.80	180.26

FILE 'CAPLUS' ENTERED AT 19:54:33 ON 20 OCT 2007
USE IS

http://www.cas.org/infopolicy.html

=> s l7
L8 4602 L7

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=> save temp ave10523964/a
ENTER L#, L# RANGE, ALL, OR (END):l8
ANSWER SET L8 HAS BEEN SAVED AS 'AVE10523964/A'

=> e us 2005-523964/apps
E1            1     US2005-52396/AP
E2            1     US2005-523963/AP
E3            1 --> US2005-523964/AP
E4            0     US2005-523964/PRN
E5            1     US2005-523965/AP
E6            1     US2005-523968/AP
E7            1     US2005-523969/AP
E8            1     US2005-52397/AP
E9            2     US2005-52397/PRN
E10           1     US2005-523971/AP
E11           1     US2005-523973/AP
E12           1     US2005-523974/AP

=> s e3
L9            1 US2005-523964/AP

=> sel rn
E1 THROUGH E252 ASSIGNED

=> fil reg
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       3.50     183.76

FILE 'REGISTRY' ENTERED AT 19:56:17 ON 20 OCT 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

http://www.cas.org/support/stngen/stndoc/properties.html

=> s e1-e252
              1 100-46-9/BI
                (100-46-9/RN)
              1 100-61-8/BI
                (100-61-8/RN)
              1 102-32-9/BI

                (97340-30-2/RN)
L10         252 (100-46-9/BI OR 100-61-8/BI OR 102-32-9/BI OR 103-82-2/BI OR
              -74-6/BI OR
               477217-75-7/BI OR 477217-76-8/BI OR 4772

=> s l10 and l7
L11          22 L10 AND L7

=> d scan

L11  22 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
IN   4H-1-Benzopyran-4-one, 3-[4-(cyclohexylamino)phenyl]-7-hydroxy-
MF   C21 H21 N O3
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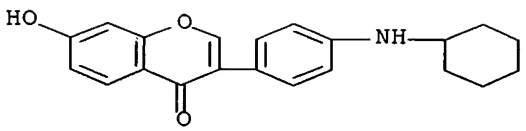

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	1.80	185.56

FILE 'CAPLUS' ENTERED AT 19:58:42 ON 20 OCT 2007

=> s l11

L12 11 L11

=> s l12 and (ay<2002 or py<2002 or pry<2002)

4190307 AY<2002
21918085 PY<2002
3667393 PRY<2002

L13 7 L12 AND (AY<2002 OR PY<2002 OR PRY<2002)

=> d ibib abs hitstr 1-7

L13 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:532647 CAPLUS Full-text
DOCUMENT NUMBER: 139:101122
TITLE: Preparation of 3,4-diarylpyrazoles as inhibitors of heat shock protein 90 (HSP90) and their use in the therapy of cancer
INVENTOR(S): Drysdale, Martin James; Dymock, Brian William; Barril-Alonso, Xavier; Workman, Paul; Pearl, Laurence Harris; Prodromou, Chrisostomos; MacDonald, Edward
PATENT ASSIGNEE(S): Ribotargets Limited, UK; Cancer Research Technology Limited; The Institute of Cancer Research
SOURCE: PCT Int. Appl., 299 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003055860	A1	20030710	WO 2002-GB5778	20021219 <--

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ,

CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2002356301	A1	20030715	AU 2002-356301	20021219 <--
EP 1456180	A1	20040915	EP 2002-805823	20021219 <--
EP 1456180	B1	20071003		

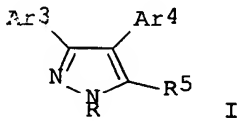
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK

JP 2005517675	T	20050616	JP 2003-556391	20021219 <--
US 2005222230	A1	20051006	US 2005-499030	20050425 <--
US 7247734	B2	20070724		

PRIORITY APPLN. INFO.:	GB 2001-30733	A	20011221 <--
	GB 2002-25688	A	20021104
	WO 2002-GB5778	W	20021219

OTHER SOURCE(S): MARPAT 139:101122

GI



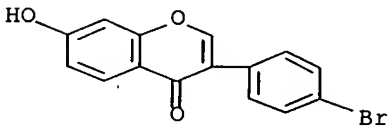
I

AB A method of inhibiting HSP90 comprises administration of title compds. [I; Ar3, Ar4 = (substituted) C5-20 aryl; R5 = H, halo, OH, ether, formyl, acyl, CO2H, ester, acyloxy, oxycarbonyloxy, amido, acylamido, aminocarbonyloxy, tetrazolyl, amino, NO2, cyano, N3, sulfhydryl, thioether, sulfonamido, C1-7 alkyl, C3-20 heterocyclyl, C5-20 aryl; R = H, C1-7 alkyl, C3-20 heterocyclyl, C5-20 aryl] and pharmaceutically acceptable salts, solvates, amides, esters, ethers, chemical protected forms, and prodrugs thereof. Thus, 7-hydroxy-3-phenylchromen-4-one and hydrazine hydrate were refluxed 45 min. in EtOH to give 4-(4-phenyl-1H-pyrazol-3- yl)benzene-1,3-diol. This inhibited HSP90 activity with IC50 = 10-100 μM.

IT 96644-05-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of diarylpyrazoles as inhibitors of heat shock protein 90 and their use in the therapy of cancer)

RN 96644-05-2 CAPLUS

CN 4H-1-Benzopyran-4-one, 3-(4-bromophenyl)-7-hydroxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:	2000:835787 CAPLUS Full-text
DOCUMENT NUMBER:	134:147420
TITLE:	1H NMR studies on synthetic isoflavones with p-substituents on B ring
AUTHOR(S):	Liu, Peng; Chen, Rong-Feng; Chang, Jun-Biao; Xie,

Jing-Xi

CORPORATE SOURCE: Henan Institute of Chemistry, Zhengzhou, 450003, Peop. Rep. China

SOURCE: Gaodeng Xuexiao Huaxue Xuebao (2000), 21(11), 1671-1674
CODEN: KTHPDM; ISSN: 0251-0790

PUBLISHER: Gaodeng Jiaoyu Chubanshe

DOCUMENT TYPE: Journal

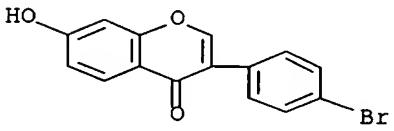
LANGUAGE: Chinese

AB In this paper, 1H NMR study on fourteen isoflavones with various p-substituents on B ring is reported. The effects of substituents on the chemical shifts of A, B and C ring protons are discussed. Unambiguous assignments of unsubstituted B ring 1H resonance spectra were made with the aid of superconductive NMR spectroanal. There is a linear relationship between the chemical shifts of B ring protons and the substituent parameters. The chemical shifts of 2'(6')-1H and 3'(5')-1H show a linear correlation with Hammett consts. σp and substituent parameter S0 resp. The resonance shifts of 3'(5')-1H arise from the electron and magnetic anisotropy effects, while the resonance shifts of 2'(6')-1H respond to the electron effects of the substituents primarily.

IT 96644-05-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(1H NMR studies on synthetic isoflavones with p-substituents on B ring)

RN 96644-05-2 CAPLUS

CN 4H-1-Benzopyran-4-one, 3-(4-bromophenyl)-7-hydroxy- (9CI) (CA INDEX NAME)



L13 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:676259 CAPLUS Full-text

DOCUMENT NUMBER: 134:246935

TITLE: Studies on synthesis and antitumor activities of soybean isoflavones and their derivatives

AUTHOR(S): Liu, Peng; Chang, Junbio; Chen, Rongfeng; Xie, Jingxi; Wang, Qiang

CORPORATE SOURCE: Henan Institute of Chemistry, Zhengzhou, 450002, Peop. Rep. China

SOURCE: Yaoxue Xuebao (2000), 35(8), 583-586
CODEN: YHHPAL; ISSN: 0513-4870

PUBLISHER: Yaoxue Xuebao Bianjibu

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

OTHER SOURCE(S): CASREACT 134:246935

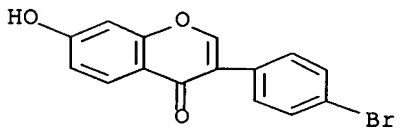
AB Thirteen deoxybenzoins and fourteen soybean isoflavones were prepared Their antitumor activities against hepatoma H22 tumor cell were tested by trypan blue exclusion method at the concentration of 50 μg mL-1. None of these compds. showed distinct antitumor activity against hepatoma H22 tumor cell, and 5,7-dihydroxy-3-(4- nitrophenyl)-4-benzopyranone and 5,7-dihydroxy-3-(4-fluorophenyl)- 4-benzopyranone gave the blue-stained ratio 10% and 5% at the concentration of 100 ng mL-1, resp.

IT 96644-05-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and antitumor activities of soybean isoflavones and their derivs.)

RN 96644-05-2 CAPLUS

CN 4H-1-Benzopyran-4-one, 3-(4-bromophenyl)-7-hydroxy- (9CI) (CA INDEX NAME)



L13 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1993:212822 CAPLUS Full-text

DOCUMENT NUMBER: 118:212822

TITLE: Formic acetic anhydride in the synthesis of chromones. 2. Synthesis of 3-arylchromones

AUTHOR(S): Pivovarenko, V. G.; Khilya, V. P.

CORPORATE SOURCE: Kiev. Gos. Univ., Kiev, 252017, Ukraine

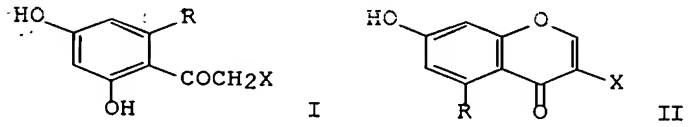
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1992), (5), 595-600
CODEN: KGSSAQ; ISSN: 0132-6244

DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 118:212822

GI

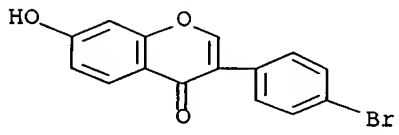


AB Dihydroxyphenylacetophenone I (R = H, X = Ph) underwent cyclization to arylchromone II (near quant. yield) in reaction with HCO2Ac via initial formylation of I under mild conditions, followed by base-catalyzed cyclization. Trialkylamines were the most effective cyclization catalysts. Et3N catalyzed the cyclization of other I derivs. (R = H, OH; X = e.g., substituted Ph or furyl) to II. The cyclization is most effectively applied to preparation of II containing electron-withdrawing X groups.

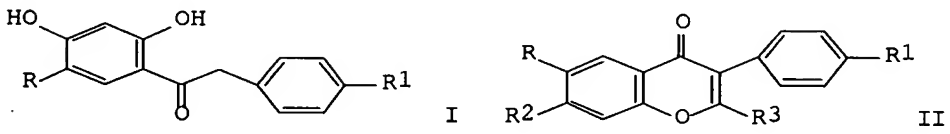
IT 96644-05-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 96644-05-2 CAPLUS

CN 4H-1-Benzopyran-4-one, 3-(4-bromophenyl)-7-hydroxy- (9CI) (CA INDEX NAME)



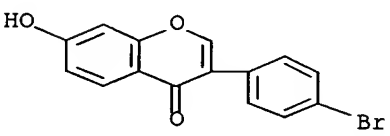
L13 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1987:66952 CAPLUS Full-text
DOCUMENT NUMBER: 106:66952
TITLE: Synthesis of analogs of natural isoflavones via 2,4-dihydroxydeoxybenzoins
AUTHOR(S): Luk'yanchikov, M. S.; Khilya, V. P.; Kazakov, A. A.
CORPORATE SOURCE: Pyatigorsk. Farm. Inst., Pyatigorsk, USSR
SOURCE: Khimiya Prirodnykh Soedinenii (1985), (6), 781-4
CODEN: KPSUAR; ISSN: 0023-1150
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 106:66952
GI



AB Condensation of 4-RC6H3(OH)2-1,3 with 4-R1C6H4CH2CN gave deoxybenzoins I (R = Et, Pr, Bu, C5H11, n-C6H13, R1 = H; R, R1 = H, Br; Et, Br; Et, Cl). These were cyclized with HC(OEt)3, (CF3CO)2O, or EtO2CCOCl to give isoflavones II (R2 = OH, R3 = H, R, R1 as above; R, R1, R2, R3 = H, Br, OH, CF3, etc.). Some of these were methylated or acetylated. II had 1.5 times the hypolipidemic activity of cetamiphen and polysponin.

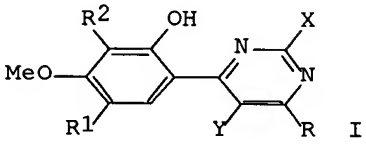
IT 96644-05-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and anticholesteremic activity of)

RN 96644-05-2 CAPLUS
CN 4H-1-Benzopyran-4-one, 3-(4-bromophenyl)-7-hydroxy- (9CI) (CA INDEX NAME)

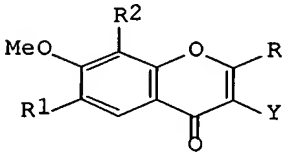


L13 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1986:608819 CAPLUS Full-text

DOCUMENT NUMBER: 105:208819
TITLE: Chemistry of isoflavone heteroanalogs. 10. Synthesis of pyrimidines by recyclization of isoflavones and their heteroanalogs
AUTHOR(S): Khilya, V. P.; Kornilov, M. Yu.; Gorbulenko, N. V.; Golubushina, G. M.; Kovtun, E. N.; Kolotusha, N. V.; Panasenko, G. V.
CORPORATE SOURCE: Kiev. Gos. Univ., Kiev, 252017, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1985), (11), 1542-50
CODEN: KGSSAQ; ISSN: 0453-8234
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 105:208819
GI

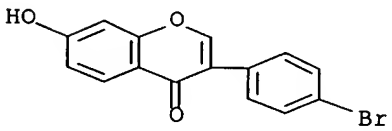


I



II

AB 4-(2-Hydroxyphenyl)pyrimidines I (R = H, Me, CF3, R1 = H, Et, Pr, hexyl, R2 = H, MeO, X = NH2, Me, H, Y = 4-thiazolyl, 2-methyl- or 2-phenyl-4-thiazolyl, Ph, substituted phenyl) were prepared in 28-86% yields by recyclization of the corresponding isoflavones II in the presence of XC(:NH)NH2.
IT 96644-05-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation of)
RN 96644-05-2 CAPLUS
CN 4H-1-Benzopyran-4-one, 3-(4-bromophenyl)-7-hydroxy- (9CI) (CA INDEX NAME)



L13 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1985:220613 CAPLUS Full-text
DOCUMENT NUMBER: 102:220613
TITLE: Synthetic analogs of natural isoflavones
AUTHOR(S): Khilya, V. P.; Luk'yanchikov, M. S.; Kazakov, A. L.; Gorbulenko, N. V.
CORPORATE SOURCE: Kiev. Gos. Univ., Kiev, USSR
SOURCE: Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1984), 50(12), 1301-6
CODEN: UKZHAU; ISSN: 0041-6045
DOCUMENT TYPE: Journal

LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 102:220613
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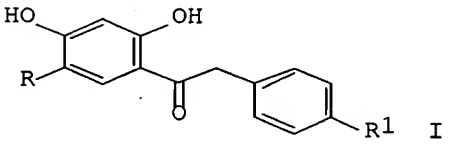

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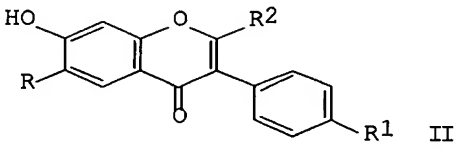


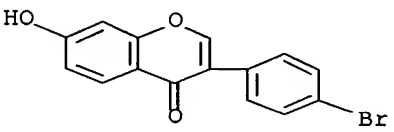
II

AB Cyclocondensation of deoxybenzoins I (R = Et, Pr, Bu, pentyl, hexyl, H; R1 = H, Br, Cl, F, NO2, MeO, Me2CHO) with HC(OEt)3, Ac2O, (F3CCO)2O, or ClCOCO2Et gave isoflavones II (R2 = H, Me, CF3, CO2Et; resp.).

IT 96644-05-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 96644-05-2 CAPLUS

CN 4H-1-Benzopyran-4-one, 3-(4-bromophenyl)-7-hydroxy- (9CI) (CA INDEX NAME)



=> d his

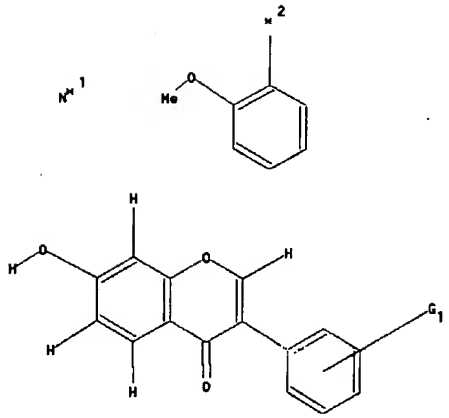
=> fil reg

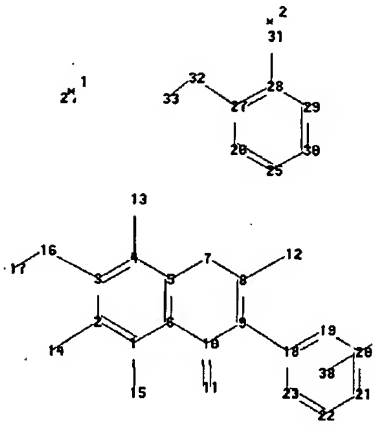
COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	52.32	237.88

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-5.46	-5.46

FILE 'REGISTRY' ENTERED AT 20:10:29 ON 20 OCT 2007

=>
Uploading C:\Program Files\Stnexp\Queries\10523964.str





chain nodes :
11 12 13 14 15 16 17 31 32 33 37
ring nodes :
1 2 3 4 5 6 7 8 9 10 18 19 20 21 22 23 25 26 27 28 29 30
ring/chain nodes :
24
chain bonds :
1-15 2-14 3-16 4-13 8-12 9-18 10-11 16-17 27-32 28-31 32-33
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 18-19 18-23 19-20 20-21
21-22 22-23 25-26 25-30 26-27 27-28 28-29 29-30
exact/norm bonds :
3-16 5-7 6-10 7-8 8-9 9-10 10-11 27-32
exact bonds :
1-15 2-14 4-13 8-12 9-18 16-17 28-31 32-33
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 18-19 18-23 19-20 20-21 21-22 22-23 25-26 25-30
26-27 27-28 28-29 29-30

G1:[*1],[*2]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:Atom
19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:Atom 26:Atom 27:Atom
28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 33:CLASS 37:CLASS 38:Atom

L14 STRUCTURE UPLOADED

=> d l14
L14 HAS NO ANSWERS
L14 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l14 sss subset=l7 sam
SAMPLE SUBSET SEARCH INITIATED 20:11:25 FILE 'REGISTRY'
SAMPLE SUBSET SCREEN SEARCH COMPLETED - 10 TO ITERATE

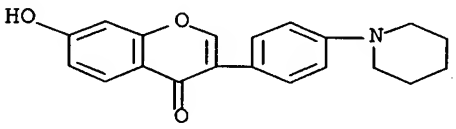
100.0% PROCESSED 10 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET): ONLINE **COMPLETE**
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET): 11 TO 389
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET): 4 TO 200

L15 4 SEA SUB=L7 SSS SAM L14

=> d scan

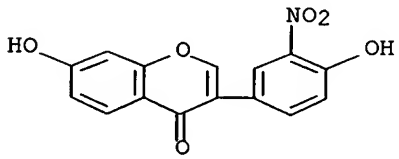
L15 4 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 4H-1-Benzopyran-4-one, 7-hydroxy-3-[4-(1-piperidinyl)phenyl]-
MF C20 H19 N O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

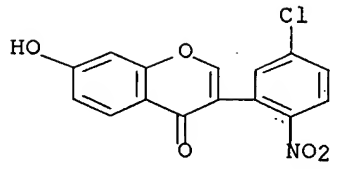
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L15 4 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxy-3-nitrophenyl)-
MF C15 H9 N O6



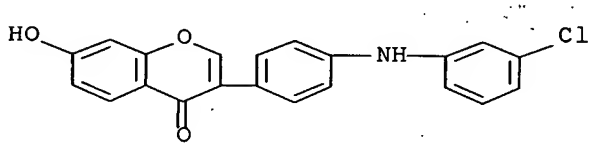
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L15 4 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 4H-1-Benzopyran-4-one, 3-(5-chloro-2-nitrophenyl)-7-hydroxy- (9CI)
MF C15 H8 Cl N O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L15 4 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 4H-1-Benzopyran-4-one, 3-[4-[(3-chlorophenyl)amino]phenyl]-7-hydroxy-
MF C21 H14 Cl N O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

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FULL SUBSET SEARCH INITIATED 20:12:15 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 289 TO ITERATE

100.0% PROCESSED 289 ITERATIONS 41 ANSWERS
SEARCH TIME: 00.00.01

L16 41 SEA SUB=L7 SSS FUL L14

=> save temp l16 av10523964/a
ANSWER SET L16 HAS BEEN SAVED AS 'AV10523964/A'

=> fil caplus
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	42.45	280.33

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-5.46

FILE 'CAPLUS' ENTERED AT 20:12:53 ON 20 OCT 2007

=> s l16
L17 36 L16

=> s l16 and (ay<2002 or py<2002 or pry<2002)

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           36 L16
      4190307 AY<2002
     21918085 PY<2002
      3667393 PRY<2002
L18         23 L16 AND (AY<2002 OR PY<2002 OR PRY<2002)

=> s l17 and (ay<2002 or py<2002 or pry<2002)
      4190307 AY<2002
     21918085 PY<2002
      3667393 PRY<2002
L19         23 L17 AND (AY<2002 OR PY<2002 OR PRY<2002)

=> d his

=> s l19 and l7
         4602 L7
L20        23 L19 AND L7

=> s l19 not l7
         4602 L7
L21         0 L19 NOT L7

=> s l19 or l7
         4602 L7
L22      4602 L19 OR L7

=> s l19 and l13
L23         3 L19 AND L13

=> s l19 not l13
L24        20 L19 NOT L13

=> s l19 or l13
L25        27 L19 OR L13

=> s l13 not l20
L26         4 L13 NOT L20

=> d ibib abs hitstr l24 1-20

L24  ANSWER 1 OF 20  CAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:        2001:239823  CAPLUS  Full-text
DOCUMENT NUMBER:         134:280704
TITLE:                   Preparation of 3-hydroxybenzoylindoles for treatment
                         of diseases associated with protein kinase and
                         estrogen activity
INVENTOR(S):             Loewe, Werner; Gust, Ronald; Witzel, Sonja; Dietrich,
                         Christoph
PATENT ASSIGNEE(S):      Germany
SOURCE:                  Ger. Offen., 12 pp.
                         CODEN: GWXXBX
DOCUMENT TYPE:           Patent
LANGUAGE:                German
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE        APPLICATION NO.          DATE
     ----------          ----   --------    --------------------     --------
     DE 19947863          A1    20010405    DE 1999-19947863         19990923 <--
PRIORITY APPLN. INFO.:                      DE 1999-19947863         19990923 <--
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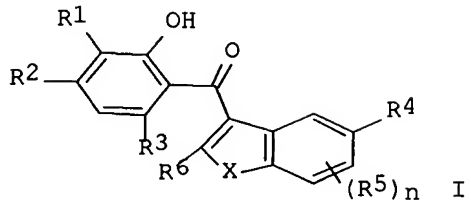
OTHER SOURCE(S): MARPAT 134:280704
GI

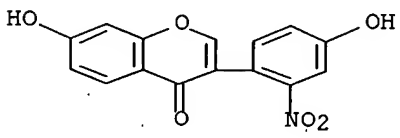


I

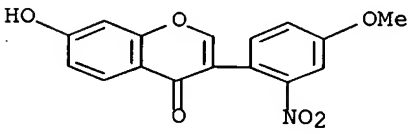
AB Use of title compds. [I; R1, R2, R3 = H, OH, alkoxy, alkyl; or R1R2 = alkylendioxy; R4 = H, halo, (halo-substituted) alkyl, OH, PhO, cycloalkyloxy, alkoxy; R5 = H, (halo-substituted) alkyl, OH, PhO, cycloalkyloxy, alkoxy; n = 0-3; R6 = H, alkyl; X = (substituted) imino] for treatment of diseases associated with protein kinase activity is claimed. Thus, 3-(2-nitrophenyl)-7-methylisoflavone (preparation from 2-nitrophenyl acetic acid given) was refluxed 20 h with Pd/C in EtOH/cyclohexane to give 54% 3-(2-hydroxy-4-methylbenzoyl)indole. The latter at 5 μM in MCF-7 cells showed a maximal cytostatic activity T/C = 10% after 160 h.

IT 332150-55-7P 332150-59-1P 332150-63-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of hydroxybenzoylindoles for treatment of diseases associated with
protein kinase and estrogen activity)

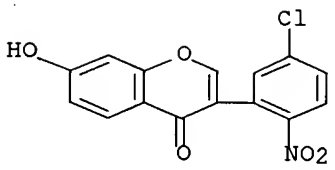
RN 332150-55-7 CAPLUS
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxy-2-nitrophenyl)- (9CI) (CA INDEX NAME)



RN 332150-59-1 CAPLUS
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-methoxy-2-nitrophenyl)- (9CI) (CA INDEX NAME)



RN 332150-63-7 CAPLUS
CN 4H-1-Benzopyran-4-one, 3-(5-chloro-2-nitrophenyl)-7-hydroxy- (9CI) (CA INDEX NAME)

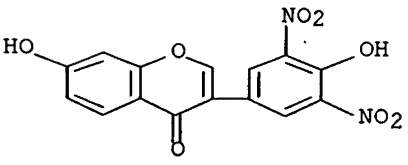


REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 2 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:735369 CAPLUS Full-text
DOCUMENT NUMBER: 132:264129
TITLE: Production, isolation and structure elucidation of novel isoflavonoid compound K3-D4, K3-D5, K3-D6
AUTHOR(S): Shangguan, Dihua; Jiang, Rong; Li, Baoyi; Xiao, Chunling; Wu, Jianbo
CORPORATE SOURCE: Institute of Medicinal Biotechnology, Peking Union Medical College, Chinese Academy of Medical Sciences, Beijing, 100050, Peop. Rep. China
SOURCE: Zhongguo Kangshengsu Zazhi (1999), 24(4), 254-257,299
CODEN: ZKZAEY; ISSN: 1001-8689
PUBLISHER: Zhongguo Kangshengsu Zazhishe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

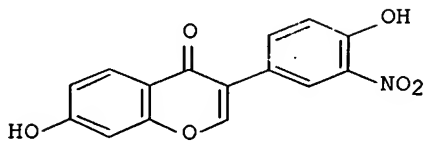
AB This thesis is on the study of lipophilic components of the genetic-engineering amikacin-producing Streptomyces K3. The fermentation broth was adjusted to pH 3 and extracted with Et acetate. By means of Sephadex LH· 20 chromatog., preparative TLC and RP-HPLC, three compds., K3-D4, K3-D5, K3-D6 resp. were isolated from the mixture of the extract By extensive study of their UV, IR, MS, 1H-NMR, 13C-NMR and HMBC spectra, the structure of K3-D4, K3-D5 and K3-D6 were elucidated. They are three novel isoflavonoids. K3-D4 was assigned to be 4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(3-nitro-4-hydroxyphenyl)-; K3-D5 was assigned to be 4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(3,5-dinitro-4-hydroxyphenyl)-; K3-D6 was assigned to be 4H-1-Benzopyran-4-one, 7-hydroxy-3-(3,5-dinitro-4- hydroxyphenyl).

IT 263554-83-2P, K 3D6
RL: BPN (Biosynthetic preparation); PRP (Properties); BIOL (Biological study); PREP (Preparation)
(production, isolation and structure elucidation of novel isoflavonoid compound K3-D4, K3-D5, K3-D6)
RN 263554-83-2 CAPLUS
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxy-3,5-dinitrophenyl)- (9CI) (CA INDEX NAME)



L24 ANSWER 3 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:683596 CAPLUS Full-text

DOCUMENT NUMBER: 127:358072
TITLE: Production, isolation and structure elucidation of new isoflavonoid compound K3-D3
AUTHOR(S): Jiang, Rong; Li, Baoyi; Xiao, Chunling; Yang, Dajun; Wu, Jianbo
CORPORATE SOURCE: Institute Medicinal Biotechnology, Peking Union Medical College, Beijing, 100050, Peop. Rep. China
SOURCE: Zhongguo Kangshengsu Zazhi (1997), 22(2), 81-83, 139
CODEN: ZKZAEY; ISSN: 1001-8689
PUBLISHER: Zhongguo Kangshengsu Zazhishe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI

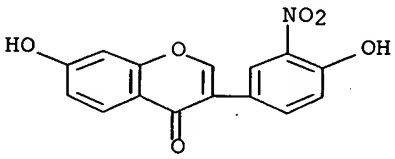


I

AB A new isoflavonoid compound K3-D3, 7,4'-2OH-3'-NO2-isoflavonoid (I) was isolated from the culture broth of a genetic-engineering Streptomyces K2. Its structure was elucidated by various NMR expts. and other spectroscopic analyses.

IT 198644-94-9P
RL: BPN (Biosynthetic preparation); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
(production, isolation and structure elucidation of new isoflavonoid compound
K3-D3)

RN 198644-94-9 CAPLUS
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxy-3-nitrophenyl)- (CA INDEX NAME)



L24 ANSWER 4 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:4560 CAPLUS Full-text
DOCUMENT NUMBER: 120:4560
TITLE: Isoflavonoid alkaloids from Piscidia erythrina
AUTHOR(S): Moriyama, Masaaki; Tahara, Satoshi; Ingham, John L.; Mizutani, Junya
CORPORATE SOURCE: Fac. Agric., Hokkaido Univ., Sapporo, 060, Japan
SOURCE: Phytochemistry (1993), 32(5), 1317-25
CODEN: PYTCAS; ISSN: 0031-9422
DOCUMENT TYPE: Journal

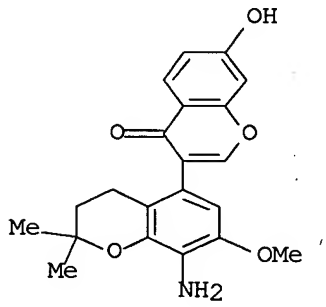
LANGUAGE: English

AB Two amino-substituted isoflavones and one with an oxazole ring were isolated from the root bark of P. erythrina. Their structures were established as 4'-amino-5,7,3'-trihydroxy-5'-methoxy-2',6'-di-(3,3- dimethylallyl)isoflavone (piscerythramine), 4'-amino-5,7,3'-trihydroxy-5'- methoxy-8,2'-di-(3,3-dimethylallyl)isoflavone (isopiscerythramine) and 7-hydroxy-5'-methoxy-2'-(3,3-dimethylallyl)-oxazolo- [4''',5''':4',3']isoflavone (piscerythoxazole) by spectroscopic and chemical methods. The first of these isoflavones was chemical converted to a compound which could also be obtained from the corresponding 4'-hydroxyisoflavone, erythbigenin.

IT 151590-47-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)

RN 151590-47-5 CAPLUS

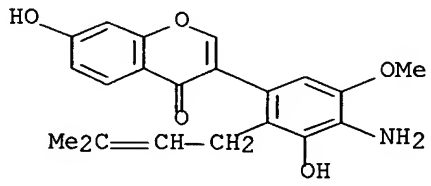
CN [3,5'-Bi-4H-1-benzopyran]-4-one, 8'-amino-2',3'-dihydro-7-hydroxy-7'-methoxy-2',2'-dimethyl- (9CI) (CA INDEX NAME)



IT 151590-46-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from piscerythoxazole)

RN 151590-46-4 CAPLUS

CN 4H-1-Benzopyran-4-one, 3-[4-amino-3-hydroxy-5-methoxy-2-(3-methyl-2-butenyl)phenyl]-7-hydroxy- (9CI) (CA INDEX NAME)



L24 ANSWER 5 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1992:6375 CAPLUS Full-text

DOCUMENT NUMBER: 116:6375

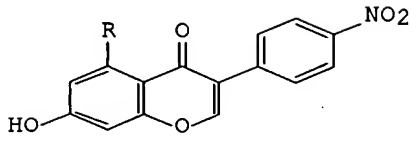
TITLE: A facile and practical preparation of 5,7-dihydroxy-3-(4-nitrophenyl)-4H-1-benzopyran-4-one

AUTHOR(S): Liu, D. F.; Cheng, C. C.

CORPORATE SOURCE: Cancer Cent., Univ. Kansas, Kansas City, KS, 66103, USA

SOURCE: Journal of Heterocyclic Chemistry (1991),

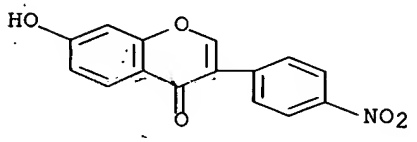
28(6), 1641-2
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:6375
GI



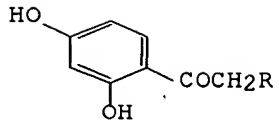
I

AB In spite of the fact that several preparative methods for the synthesis of hydroxylated isoflavones were reported during the past fifty years, none is suitable for the preparation of isoflavones containing 5,7-dihydroxy functions. This paper reports a simple, large scale preparation of 5,7-dihydroxy-3-(4- nitrophenyl)-4H-1-benzopyran-4-one (I, R = OH) by the condensation of the readily available 2,4,6-(HO)3C6H2COCH2C6H4NO2-4 and acetic formic anhydride in high yields. Similar isoflavones, such as I (R = H), can also be obtained in good yields in an analogous manner.

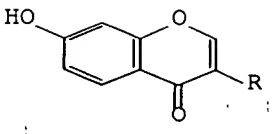
IT 15485-80-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 15485-80-0 CAPLUS
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-nitrophenyl)- (CA INDEX NAME)



L24 ANSWER 6 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1990:405988 CAPLUS Full-text
DOCUMENT NUMBER: 113:5988
TITLE: Simple and effective synthesis of isoflavones and 3-arylhydroxychromones
AUTHOR(S): Pivovarenko, V. G.; Khilya, V. P.; Vasil'ev, S. A.
CORPORATE SOURCE: Kiev. Gos. Univ., Kiev, USSR
SOURCE: Khimiya Prirodnykh Soedinenii (1989), (5), 639-43
CODEN: KPSUAR; ISSN: 0023-1150
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 113:5988
GI



I



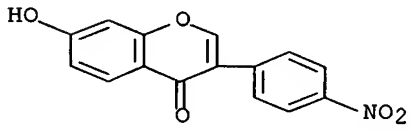
II

AB Cyclocondensation of acetophenones I (R = substituted Ph, PhO, p-FC6H4O) with MeCO2CHO, prepared from HCO2H and CH2:C:O, gave 15-99% isoflavones II. Similarly, I react with the Vilsmeier reagent to give 95.7-98.5% II.

IT 15485-80-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 15485-80-0 CAPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-nitrophenyl)- (CA INDEX NAME)



L24 ANSWER 7 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1985:541792 CAPLUS Full-text

DOCUMENT NUMBER: 103:141792

TITLE: Acetic formic anhydride as a cyclizing reagent in the synthesis of isoflavones and 3-hetarylchromones

AUTHOR(S): Pivovarenko, V. G.; Khilya, V. P.; Babichev, F. S.

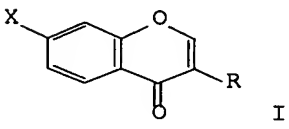
CORPORATE SOURCE: Kiiv. Derzh. Univ., Kiev, USSR

SOURCE: Dopovidi Akademii Nauk Ukrains'koi RSR, Seriya B: Geologichni, Khimichni ta Biologichni Nauki (1985), (4), 56-9
CODEN: DANND6; ISSN: 0377-9785

DOCUMENT TYPE: Journal

LANGUAGE: Ukrainian

GI

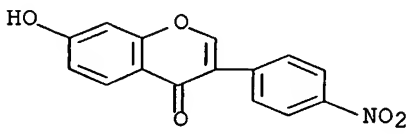


I

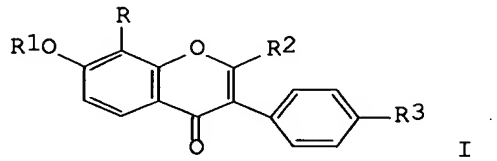
AB HCO2Ac catalyzed the cyclization of 2,4-(HO)2C8H4COCH2R [R = 2-pyridyl, 2- and 7-quinolyl, 2-methyl-4-thiazolyl, 5-(ethoxycarbonyl)-2-furyl, C6H4NO2-4, Ph, C6H4OMe-4, Me] in the presence of NaO2CH or Et3N to give ≤99% chromones I (X = HO, same R). The intermediate I (X = HCO2; R = 2-pyridyl, 2-quinolyl, 2-methyl-4-thiazolyl) were also isolated.

IT 15485-80-0P
RL: SPN (Synthetic preparation); PREP (Preparation)

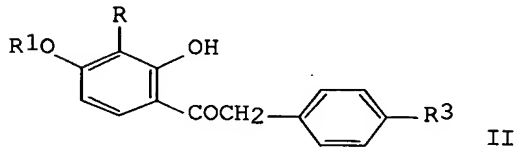
(preparation of, by cyclization of dihydroxyacetophenone derivative, catalysts
for)
RN 15485-80-0 CAPLUS
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-nitrophenyl)- (CA INDEX NAME)



L24 ANSWER 8 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1981:174809 CAPLUS Full-text
DOCUMENT NUMBER: 94:174809
TITLE: Studies on the synthesis and structure-antihypoxia activity relations of daidzein, an active principle of Pueraria pseudohiruta, and its derivatives
AUTHOR(S): Shao, Guo-Xian; Mo, Ruo-Ying; Wang, Cun-Ying; Zhang, De-Yong; Yin, Zhong-Zhu; Ouyang, Rong; Xu, Li-Na
CORPORATE SOURCE: Inst. Materia Med., Chin. Acad. Med. Sci., Peking, Peop. Rep. China
SOURCE: Yaoxue Xuebao (1980), 15(9), 538-47
CODEN: YHHPAL; ISSN: 0513-4870
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI

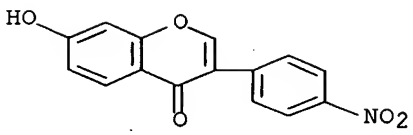


I

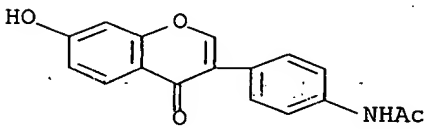


II

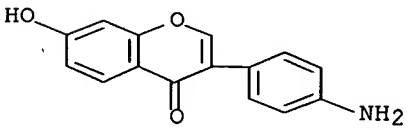
AB Daidzein (I, R-R2 = H, R3 = OH) and its analogs I (R = H, OH; R1 = H, alkyl, acyl; R2 = H, Me; R3 = H, OH, OMe, Cl, NO2, NH2,NHAc, OCH2CO2Et) were prepared by condensing II with HCO2Et and Ac2O. The antihypoxia activity of I (R, R1, R2, R3 = H, H, H, OMe; H, Me, H, OMe; H, CH2CO2Et, H, OCH2CO2Et) is more potent than that of daidzein.
IT 15485-80-0P 77316-77-9P 77316-78-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antihypoxia activity of)
RN 15485-80-0 CAPLUS
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-nitrophenyl)- (CA INDEX NAME)



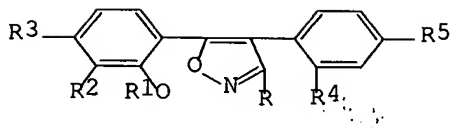
RN 77316-77-9 CAPLUS
CN Acetamide, N-[4-(7-hydroxy-4-oxo-4H-1-benzopyran-3-yl)phenyl]- (9CI) (CA INDEX NAME)



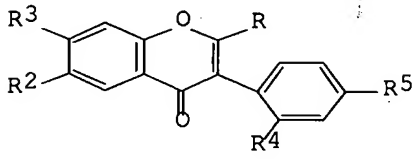
RN 77316-78-0 CAPLUS
CN 4H-1-Benzopyran-4-one, 3-(4-aminophenyl)-7-hydroxy- (9CI) (CA INDEX NAME)



L24 ANSWER 9 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1981:156800 CAPLUS Full-text
DOCUMENT NUMBER: 94:156800
TITLE: Synthesis of 4,5-diphenylisoxazoles and their insecticidal derivatives
AUTHOR(S): Borda, J.; Szabo, V.; Nemeth, L.; Bokor, G.
CORPORATE SOURCE: Inst. Appl. Chem., Kossuth Lajos Univ., Debrecen, Hung.
SOURCE: Acta Chimica Academiae Scientiarum Hungaricae (1980), 104(4), 389-96
CODEN: ACASA2; ISSN: 0001-5407
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



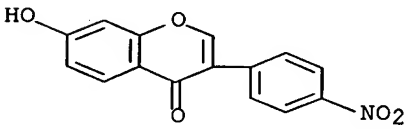
II

AB Isoxazoles I (R = H, Me, CF3; R1 = H; R2 = H, Me; R3 = H, OH, OMe; R4 = H, OMe; R5 = H, OMe, NO2) were prepared in 69.7-92.8% yield by reacttion of chromones II with NH2OH. Treatment of I (R1 = H) with R6NCO (R6 = Me, Et, Bu) gave I (R1 = CONHR6). I [R = H, Me, CF3; R1 = P(S)(OEt)2; R2-R5 = H] were similarly prepared I [R = H, Me, CF3; R1 = CONHR6, P(S)(OEt)2; R2-R5 = H] had insecticidal activity (no data).

IT 15485-80-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with hydroxylamine)

RN 15485-80-0 CAPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-nitrophenyl)- (CA INDEX NAME)



L24 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1981:103116 CAPLUS Full-text

DOCUMENT NUMBER: 94:103116

TITLE: Ring transformation of chromones into 4-hydroxycoumarins

AUTHOR(S): Szabo, Vince; Borda, Jeno; Theisz, Edit

CORPORATE SOURCE: Inst. Appl. Chem., Kossuth Lajos Univ., Debrecen, H-4010, Hung.

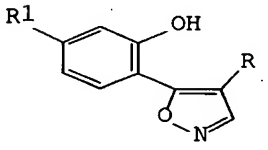
SOURCE: Acta Chimica Academiae Scientiarum Hungaricae (1980), 103(3), 271-9
CODEN: ACASA2; ISSN: 0001-5407

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 94:103116

GI



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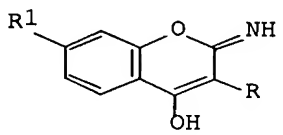


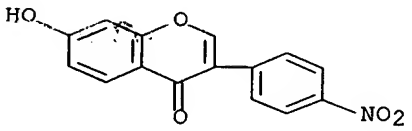
III

AB The reaction of chromone and its C-3 substituted analogs with HONH2 in aqueous solution gave the oxazoles I (R = H, Me, Ph, p-MeOC6H4, p-O2NC6H4; R1 = H, MeO, HO) via 4,2-R1(HO)C6H3COCHRCH:NOH (II). Under alkaline conditions both I and II were transformed into 4,2-R1(HO)C6H3COCHRCN, which is in a ring-chain tautomeric equilibrium with coumarin imine III, dependent on reaction conditions. III was converted into the corresponding 4-hydroxycoumarins.

IT 15485-80-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with hydroxylamine)

RN 15485-80-0 CAPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-nitrophenyl)- (CA INDEX NAME)



L24 ANSWER 11 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1978:508952 CAPLUS Full-text

DOCUMENT NUMBER: 89:108952

TITLE: Ring transformation of chromones into 4-hydroxy-coumarins

AUTHOR(S): Szabo, V.; Borda, J.

CORPORATE SOURCE: Inst. Angew. Chem., Kossuth L. Univ., Debrecen, Hung.

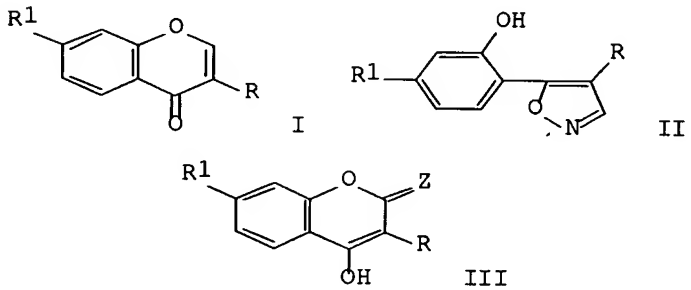
SOURCE: Acta Chimica Academiae Scientiarum Hungaricae (1977), 95(2-3), 333-4
CODEN: ACASA2; ISSN: 0001-5407

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 89:108952

GI



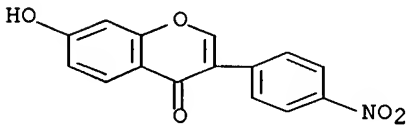
AB The chromones I (R = H, Me, Ph, 4-O2NC6H4, 4-MeOC6H4; R1 = H, HO, MeO) reacted with HONH2 to give the isoxazoles II which upon treatment with 1-4 M NaOH gave 2,4-(HO)R1C6H3COCHRCN or III (Z = NH), depending on the pH of the reaction

medium. Hydrolysis of III (Z = NH) gave III (Z = O), thus providing a new pathway from chromones to 4-hydroxycoumarin.

IT 15485-80-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with hydroxylamine, hydroxyphenylisoxazole from)

RN 15485-80-0 CAPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-nitrophenyl)- (CA INDEX NAME)



L24 ANSWER 12 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1974:47786 CAPLUS Full-text

DOCUMENT NUMBER: 80:47786

TITLE: Synthesis of isoflavone derivative. Syntheses of 7-hydroxy-2'-methoxy-5'-nitroisoflavone and related compounds

AUTHOR(S): Fukushima, Seigo; Kinoshita, Masaharu; Noro, Tadataka

CORPORATE SOURCE: Shizuoka Coll. Pharm., Shizuoka, Japan

SOURCE: Yakugaku Zasshi (1973), 93(11), 1514-16
CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

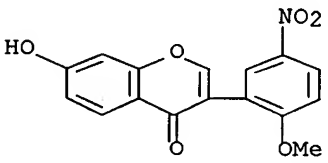
GI For diagram(s), see printed CA Issue.

AB ω-(2-Methoxy-5-nitrophenyl)-2,4-dihydroxyacetophenone, ω-(2-methoxy-5-nitrophenyl)-2,4-dimethoxyacetophenone, and 7-hydroxy-2'-methoxy-5'-nitroisoflavone (I) were prepared, by condensation of 3-ROC6H4OR (R = H, Me) with 2,5-(MeO)O2NC6H3CH2CO2H.

IT 51073-07-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 51073-07-5 CAPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(2-methoxy-5-nitrophenyl)- (9CI) (CA INDEX NAME)



L24 ANSWER 13 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1968:477068 CAPLUS Full-text

DOCUMENT NUMBER: 69:77068

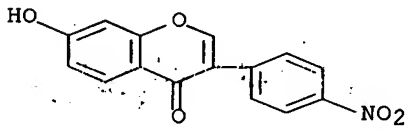
ORIGINAL REFERENCE NO.: 69:14403a,14406a

TITLE: Studies in isoflavones. I. Bromination, iodination, and nitration of 7-hydroxyisoflavone

AUTHOR(S): Chudgar, N. K.; Mani, N. V.; Sethna, Suresh

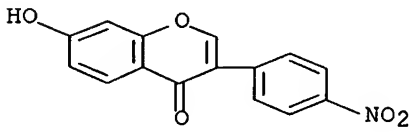
CORPORATE SOURCE: M. S. Univ. Baroda, Baroda, India

SOURCE: Journal of the Institution of Chemists (India) (1967), 39(5), 203-8
CODEN: JOICA7; ISSN: 0020-3254
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Various substitution reactions of benzo-α- and -γ-pyrone derivs. were studied by brominating, iodinating, and nitrating 7-hydroxyisoflavone (I) to see the pattern of substitution and to prepare intermediates for further synthetic work. Bromination of I with 1 mole Br gave the 8-bromo derivative, which on methylation and subsequent hydrolysis gave 2-hydroxy-4-methoxy-3-bromophenyl benzyl ketone. With 4 moles Br, I gave the 6,8-dibromo derivs. which on methylation and hydrolysis gave 2-hydroxy-4-methoxy-3,5-dibromophenyl benzyl ketone. With liquid Br, I gave 7-hydroxy-2,6,8-tribromoisoflavone (II), and hydrolysis of its Me ether gave 2-hydroxy-4-methoxy-3,5-dibromophenyl benzyl ketone and benzoic acid. Iodination of I with 1 mol. iodine and iodic acid, or with iodine and NH3, gave the 8-iodo derivative, which on methylation and subsequent hydrolysis gave 2-hydroxy-4-methoxy-3-iodophenyl benzyl ketone. With excess iodine and iodic acid, I gave 7-hydroxy-6,8-diiodoisoflavone. On nitration with fuming HNO3 in HOAc, I gave the 8-nitro derivative, and on nitration with a mixture of HNO3 and H2SO4 at 0-5°, the Me ether of I gave the 4'-nitro derivative Nitration of I with a mixture of HNO3 and H2SO4 at 5-10° gave the 4',8-dinitro derivative (III), identical with the product obtained on nitration of 7-methoxy-8-nitro- and 7-methoxy-4'-nitroisoflavone with the same mixture at 5-10°.
IT 15485-80-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 15485-80-0 CAPLUS
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-nitrophenyl)- (CA INDEX NAME)



L24 ANSWER 14 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1967:84305 CAPLUS Full-text
DOCUMENT NUMBER: 66:84305
ORIGINAL REFERENCE NO.: 66:15759a,15762a
TITLE: Antifertility activity of isoflavones related to genistein
AUTHOR(S): Moersch, George W.; Morrow, Duane F.; Neuklis, Winifred A.
CORPORATE SOURCE: Res. Labs., Parke, Davis and Co., Ann Arbor, MI, USA
SOURCE: Journal of Medicinal Chemistry (1967), 10(2), 154-8
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A group of 35 isoflavones has been synthesized by known procedures. They were tested for antifertility effects in a mouse litter prevention assay and as hypocholesteremic agents in normal rats. Only low orders of activity were found for any of the compds. Relations between structure and activity are discussed. 14 references.

IT 15485-80-0
RL: BIOL (Biological study)
(antifertility and cholesterol-lowering activity of)
RN 15485-80-0 CAPLUS
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-nitrophenyl)- (CA INDEX NAME)



L24 ANSWER 15 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1962:12914 CAPLUS Full-text
DOCUMENT NUMBER: 56:12914
ORIGINAL REFERENCE NO.: 56:2408d-i,2409a-d
TITLE: Chromones. XXXIII. Further applications of the ethyl orthoformate method for the synthesis of isoflavones
AUTHOR(S): Karmarkar, S. S.
CORPORATE SOURCE: Univ. Bombay
SOURCE: Journal of Scientific & Industrial Research (1961), 20B, 334-8
CODEN: JSIRAC; ISSN: 0022-4456
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

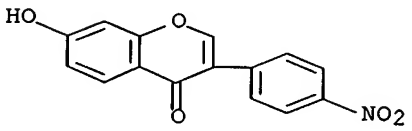
AB cf. CA 51, 5059e. A nitro substituent in the para position of the benzyl group mildly increased the reactivity of the CH2 group in condensations with Et orthoformate (Ia), but isoflavone yield depended more on the nature and position of the substituents in the o-hydroxyphenyl half of deoxybenzoin. Protection of the OH groups (e.g., by methylation), other than the one required for cyclization, improved the yield of isoflavones from Ia, C5H5N, piperidine, and deoxybenzoins derived from phloroglucinol. PhCH2CO2H (5 g.) in 20 ml. dry alc.-free CHCl3, ice-cold, was saturated with BF3 gas. Resorcinol (2.5 g.) was added to the separated material. The mixture was resatd. with BF3 gas, left overnight at room temperature, poured over ice, and extracted with ether. The ether-CHCl3 layer was washed (NaHCO3 solution, H2O) and dried (Na2SO4) and the solvent evaporated to give 4.5 g. benzyl 2,4-dihydroxyphenyl ketone (I), m. 115° (alc.). I (1 g.) was refluxed with 2 ml. C5H5N, 1.9 ml. Ia, and 2 drops piperidine. A solid separated after approx. 1 hr.; the mixture was cooled, poured over ice and HCl, kept overnight, and filtered to give 0.85 g. 7-hydroxyisoflavone (II), m. 210°(alc.). The BF3 method was used to prepare 0.15 g. 2,4-dihydroxyphenyl 4-nitrobenzyl ketone (III), m. 210° (dilute alc.), from 1 g. p-NO2C6H4CH2CO2H and 0.5 g. resorcinol in CHCl3. III (0.2 g.) was treated with 1.6 ml. C5H5N, 0.35 ml. Ia, and 2 drops piperidine and refluxed 45 min. to precipitate 0.19 g. 7-hydroxy-4'- nitroisoflavone (IV), m. 290° (alc. or glacial HOAc). IV (0.2 g.) was added to a suspension of 0.3 g. Zn dust and 20 ml. alc., 4 ml. HOAc added gradually (2 hrs.) to the refluxing solution, and heating continued 1 hr. The mixture was filtered hot and the filtrate concentrated to approx. 5 ml. and diluted with H2O to precipitate 0.13 g. 7-hydroxy-4'-aminoisoflavone (V), m. 265-6° (dilute alc.). V (0.2 g.) was dissolved in 1.5 ml. H2O and 2 ml. concentrated H2SO4, the solution cooled with ice and treated with 0.1 g. NaNO2, the mixture kept 30 min. at 0°, and excess HNO2 destroyed by the addition of urea. The solution was poured into a boiling mixture of 15 ml. H2O and 5 ml. concentrated H2SO4 and boiling continued until the solution did not give color with alkaline β-naphthol. The solution was cooled to precipitate 0.14 g. 4',7-

dihydroisoflavone (VI), m. 320°(alc.), after purification by acetylation. The diethyl ether of VI, yellow, m. 134 (dilute alc.) was prepared by refluxing VI 12 hrs. with Me2CO, K2CO3, and Et2SO4. IV was methylated by using K2CO3, Me2CO, and Me2SO4. 7-Methoxy-4'- nitroisoflavone (VII) m. 245° (dilute HOAc). VII (0.2 g.) was suspended in 50 ml. alc. with 0.5 g. Zn dust and refluxed 15 min. Glacial HOAc (4 ml.) was added during 2 hrs., heating continued 30 min., and the product filtered hot. The filtrate was concentrated, diluted with H2O, and cooled to precipitate 0.14 g. 7-methoxy-4'-aminoisoflavone (VIII), pale yellow, m. 206° (alc.). VIII (0.15 g.) was diazotized, the product hydrolyzed, the precipitate obtained treated with NaOH, the solution filtered, and the filtrate acidified to give 0.07 g. 7-methoxy-4'-hydroxyisoflavone (IX), pale yellow, m. 216-18° on remelting (aqueous alc.). 2,4-Dihydroxyphenyl 4-methoxybenzyl ketone (X) (0.6 g.), m. 159° (dih alc.), was prepared from 1.0 g. p-methoxyphenylacetic acid and 0.5 g. resorcinol in 15 ml. alc.-free CHCl3 by the BF, procedure. X was refluxed 2 hrs. with 2 ml. C5H5N, 0.5 ml. Ia, and 2 drops piperidine to yield 0.072 g. 7-hydroxy-4'-methoxyisoflavone, m. 257° (alc.). PhCH2CO2H (12 g.) and 6 g. pyrogallol, by the BF3 procedure, gave benzyl 2,3,4-trihydroxyphenyl ketone (XI), m. 140-1° (alc.): XI (1 g.), 4 ml. C5H5N, 0.8 ml. piperidine, and 1.8 mh Ia refluxed 1 hr., cooled, poured over ice and HCl, and kept overnight precipitated 0.7 g. 7,8-dihydroxyisoflavone (XII), m. 216° (alc.). XII, dried in vacuo 3 hrs. at 150° over P2O5, m. 219°; Ac derivative m. 137-9° (dilute alc.). Also prepd, were 2,3,4-trihydroxyphenyl 4-nitrobenzyl ketone, m. 227-8°; 7,8-dihydroxy-4'nitroisoflavone, yellow, m. 325° (decomposition) (glacial HOAc); 2,3,4-trihydroxyphenyl 4-methoxybenzyl ketone, m. 145-6° (aqueous alc.); 7,8-dihydroxy-4'- methoxyisoflavone, pale yellowish brown, m. 249° (aqueous ale.); 4',7,8-trihydroxyisoflavone, m. 210° (aqueous alc.) [tri-Ac deriv, m. 192° (aqueous alc.)]; 2,6-dihydroxy-4-methoxy-m-tolyl 4-nitrobenzyl ketone, m. 201° (alc.); 7-hydroxy-5-methoxy-8-methyl-4'- nitroisoflavone, yellow, decomposing above 320° (glacial HOAc); 3-carbo-methoxy- 2,4,6- trihydroxyphenyl 4-nitrobenzyl ketone, cream, m. 185-6° (alc.); 3-carbomethoxy-2-hydroxy-4,6dimethoxyphenyl 4-nitrobenzyl ketone, m. 173-4° (dilute HOAc); 8-carbomethoxy-5,7- dimethoxy-4'-nitroisoflavone, cream, m. 179-80° (alc.). 17 references.

IT 15485-80-0P, Isoflavone, 7-hydroxy-4'-nitro-
RL: PREP (Preparation)
(preparation of)

RN 15485-80-0 CAPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-nitrophenyl)- (CA INDEX NAME)



L24 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1961:68850 CAPLUS Full-text

DOCUMENT NUMBER: 55:68850

ORIGINAL REFERENCE NO.: 55:13050a-e

TITLE: Ultraviolet absorption spectra of isoflavones

AUTHOR(S): Bognar, R.; Szabo, V.; David, R. E.

CORPORATE SOURCE: L. Kossuth Univ., Debrecen, Hung.

SOURCE: Acta Univ. Szegediensis, Acta Phys. et Chem. (1959), 5, 6-18

DOCUMENT TYPE: Journal

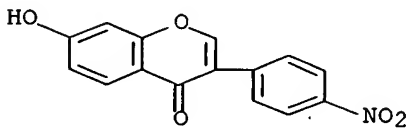
LANGUAGE: German

AB Ultraviolet spectra were given for the EtOH solns. of flavone, isoflavone, 7-methoxy-, 7-hydroxy-, 7,4'-dihydroxy-, 7-hydroxy-4'-methoxy-, 7-methoxy-4'-hydroxy-, 7-methoxy-4'-amino, 7-hydroxy-4'-amino-, 7-hydroxy-4'-nitro-, 5,7,4'-trihydroxy-, 5,7,4'-trimethoxy-, 5,4'-dihydroxy-7-methoxy-, 5,7,4'-trihydroxy-2-carbethoxy-, and 5,7,4'-trihydroxy-2-carboxyisoflavone. Isoflavone exhibited a weak band at 3080 A. (Band I) and a much stronger, sym. band at 2450 A. (Band II). Band I was assigned to the conjugation system of the ortho-condensed aromatic ring with the C:O of the 4-pyrone ring and Band II to the 4-pyrone ring system. Flavone had bands at similar locations, but relative intensities were reversed. Spectra for the first 3 compds. in cyclohexane solution were similar to those in EtOH, but intensities were lower. An electron-donor group substituted on the C7 atom of isoflavone increased the intensity of Band I and caused spreading of Band II. Addnl. substitution on the C4' atom spread Band II further and shifted it toward the visible. With NH2 substitution, splitting of Band II was complete and Band III appeared at 2700 A. This was assigned to conjugation of the other aromatic ring with the 4-pyrone ring. With addnl. substitution on the C5 atom a single, wide, asym. band of high intensity occurred at about 2620 A. Further substitution on the C2 atom (as in the last 2 compds.) decreased the intensity of the band by hindering resonance. Spectra of both acid and basic solns. of several of the compds. showed marked differences for OH- and NH2-substituted compds. as compared with neutral solution The electron-donor ability of OH was increased in basic EtOH and that of NH2 was destroyed by salt formation in acid EtOH.

IT 15485-80-0, Isoflavone, 7-hydroxy-4'-nitro-
(spectrum of)

RN 15485-80-0 CAPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-nitrophenyl)- (CA INDEX NAME)



L24 ANSWER 17 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1955:1302 CAPLUS Full-text

DOCUMENT NUMBER: 49:1302

ORIGINAL REFERENCE NO.: 49:301h-i,302a-i,303a-i

TITLE: A new synthesis of isoflavones. I

AUTHOR(S): Baker, Wilson; Chadderton, J.; Harborne, J. B.; Ollis, W. D.

CORPORATE SOURCE: Univ. Bristol, UK

SOURCE: Journal of the Chemical Society (1953) 1852-60
CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 49:1302

AB Benzyl 2-hydroxyphenyl ketones react at room temperature with ClCOCO2Et (I) in C5H5N to give 2-carbethoxyisoflavones. Hydrolysis and decarboxylation give the isoflavones. To the benzyl-2-hydroxyphenyl ketone in ice-cold C5H5N (10 ml./g.) is slowly added redistd. I [(n + 1) equivs. for a ketone with n phenolic groups] with shaking, the mixture poured the next day into H2O, extracted with CHCl3, the organic layer washed with 10% HCl, dried (MgSO4), evaporated, and the product crystallized from EtOH (in some cases, dried over P2O5 to remove traces of C5H5N). The following 2-carbethoxy-isoflavones were

so prepared from the indicated ketones. 2,4-(HO)2C6H3COCH2Ph gives 31% 7-HO compound (II), plates, m. 211.5° (acetate, m. 76-7°). 2,4-Dihydroxyphenyl 3,4-methylenedioxybenzyl ketone gives 75% 7-hydroxy-3',4'-methylenedioxy compound, yellow needles, m. 253° (acetate, m. 170°). 2,4-Dihydroxyphenyl 4-methoxybenzyl ketone yields 76% 7-hydroxy-4'-methoxy derivative, m. 209-10° (acetate, m. 123°). 2,4-Dihydroxyphenyl 4-hydroxybenzyl ketone gives 50% 4',7-di-HO compound, m. 194-5° (from aqueous EtOH) (diacetate, m. 145°). 2,4-Dihydroxyphenyl 4-nitrobenzyl ketone gives 40% 7-hydroxy-4'-nitro compound, m. 229° (acetate, m. 143°). 3,4-Methylenedioxybenzyl 2,4,6-trihydroxyphenyl ketone, needles, m. 202°, formed in 65% yield by a Hoesch reaction from phloroglucinol and 3,4-CH2O2C6H3CH2CN, gives 87% 5,7-dihydroxy-3',4'-methylenedioxy compound, yellow needles, m. 223° (from aqueous EtOH) (diacetate, m. 158-9°). 2,4,6-(HO)3C6H2COCH2Ph ketone gives 45% 5,7-di-HO compound (IIA), light yellow needles, m. 230° (diacetate, m. 153-4°). 4-Hydroxybenzyl 2,4,6-trihydroxyphenyl ketone gives 55% 4',5,7-tri-HO compound, yellow prisms, m. 240-2° (decomposition) (triacetate, m. 181-3°). 4-Methoxybenzyl 2,4,6-trihydroxyphenyl ketone gives 60% 5,7-dihydroxy-4'-methoxy compound, pale yellow needles (from C6H6), m. 189-90° (diacetate, m. 166-7°; di-Me ether, m. 150-1°). 4-Nitrobenzyl 2,4,6-trihydroxyphenyl ketone gives 52% 5,7-dihydroxy-4'-nitro compound, yellow plates (from aqueous EtOH), m. 190-1° (diacetate, m. 210-11°). The carbethoxy derivs. were hydrolyzed by either (a) adding 2N NaOH (1 equivalent for each phenolic group and 1 for the ester) to an Me2CO solution of the ester with enough H2O to clarify the solution, evaporating the Me2CO after 24 hrs. at room temperature, and acidifying the solution, or (b) warming the ester in Me2CO or EtOH 3-4 hrs. with excess 5% Na2CO3 solution, evaporating the solvent, and acidifying the solution In either case the solid acid is collected, washed with water, and dried (some contain H2O of crystallization). The acids are decarboxylated by heating in vacuo in a sublimation apparatus (the isoflavones sublime), or, better, by heating rapidly in about 50-mg. portions some 10° above the m.p. until the evolution of CO2 ceases (2-5 min.). The crude melt is crystallized and washed with a NaHCO3 solution, or purified through the Ac derivative Thus were obtained the following compds. (% yield and m.p. given): 7-hydroxyisofiavone-2-carboxylic acid, 80, needles from aqueous EtOH, 247° (decomposition); 7-hydroxy-isoflavone, 75, prisms, 213°; 7-hydroxy-3',4'-methylene-dioxyisoflavone-2-carboxylic acid, 70, 275°; 7-hydroxy-3', 4'-methylenedioxyisoflavone (ψ-baptigenin), 61, yellow crystals from aqueous EtOH, 292° (acetate, m. 165°); 7-hydroxy-4'-methoxyisoflavone-2-carboxylic acid, 98, 238°; 7-hydroxy-4'-methoxyisoflavone (formononetin), 91, plates, 257° (acetate, m. 166°); 4',7-dihydroxyisoflavone-2-carboxylic acid, 88, 290°; 4',7-dihydroxyisoflavone (daidzein), 98, needles, 320-28° (decomposition) (diacetate, m. 189°); 7-hydroxy-4'-nitroisoflavone-2-carboxylic acid, 99, 252°; 7-hydroxy-4'-nitroisoflavone, 98, needles, 292° (acetate, m. 222-3°); 5,7-dihydroxy-3',4'-methylenedioxyisoflavone-2-carboxylic acid, 90, 264°; 5,7-dihydroxy-3',4'-methylene-dioxyisoflavone, 8 (by sublimation), pale yellow needles from aqueous EtOH, 227° (diacetate, m. 216°); 5,7-dihydroxyisoflavone-2-carboxylic acid, 76, yellow needles from aqueous EtOH, 255° (decomposition); 5,7-dihydroxyisoflavone, 25 (by sublimation), plates from C6H6, 195-6° (diacetate, m. 173-4°); 4',5,7-trihydroxyisoflavone-2-carboxylic acid, 84, 310°, decarboxylated and acetylated to 4',5,7-triacetoxyisoflavone, 21, 195-8° which on hydrolysis (aqueous EtOHNa2CO3) gives 4',5,7-trihydroxyisoflavone (genistein), 88, needles, 296° (decomposition); 5,7-dihydroxy-4'-methoxyisoflavone-2-carboxylic acid, 98, m. 276°, decarboxylated and acetylated to 5,7-diacetoxy-4'-methoxyisoflavone, 81, 189-90°, which on hydrolysis gives the 5,7-di-HO compound (biochanin-A), 61, needles (from aqueous EtOH), 211-12°; 5,7-dihydroxy-4'-nitroisoflavone-2-carboxylic acid, 87, 260°; 5,7-dihydroxy-4'-nitroisoflavone, 23 (by sublimation), yellow needles, 294-5° (diacetate, m. 212-13°; di-Me ether, m. 220-1°). The Hoesch reaction between 7.6 g. 3,5-(HO)2C6H3OMe and 7.3 g. p-HOC6H4CH2CN (III) gives 8.5 g. 2,4-dihydroxy-6-methoxyphenyl 4-hydroxybenzyl

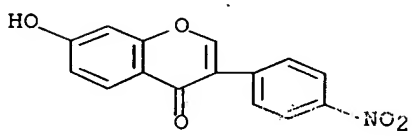
ketone (IV), needles from aqueous EtOH, m. 186-8°. IV in C5H5N treated at 0° with I gives 2-carbethoxy-4',7-dihydroxy-5- methoxyisoflavone (V) separating at the interface, which yields 10% cubes from aqueous MeOH, m. 223-4°. V hydrolyzed [the acid (83%), m. 254-5°] and decarboxylated gives 4',7-dihydroxy-5- methoxyisoflavone, 51, needles from aqueous EtOH, 316° (decomposition) (diacetate, needles, m. 168-70°). III and BzCl in C5H5N give 4-BzOC6H4CH2CN (VI), 84, needles, 106-8°. The Hoesch reaction between VI and phloroglucinol gives 4-benzoyloxybenzyl 2,4,6-trihydroxyphenyl ketone, 44, needles from aqueous EtOH, 224° (decomposition), 3 g. of which with I in C5H5N at 0° yields 2.48 g. 4'-benzoyloxy-2-carbethoxy-5,7-dihydroxyisoflavone (VII), yellow plates from MeOH, m. 248° (decomposition) [diacetate, plates from Me2CO, m. 232°]. VII (1.12 g.), 150 ml. C6H6, 5 g. ignited K2CO3, and 0.27 ml. Me2SO4 kept 2 hrs. at 100° give 4'-benzoyloxy-2-carbethoxy-5- hydroxy-7-methoxyisoflavone, 80, pale yellow plates from Me2CO, 202-4°, which on hydrolysis gives 4',5-dihydroxy-7- methoxyisoflavone-2-carboxylic acid, 97, 270°, decarboxylated to 4',5-dihydroxy-7-methoxyisoflavone (prunetin), 63, needles from MeOH, 236° (diacetate, m. 218-20°). I added with shaking to sublimed o-HOC6H4COCH2Ph in C5H5N and the mixture poured into 100 ml. HOAc after 24 hrs. gives 2-carbethoxy-2'-hydroxyisoflavanone (VIII), 83, plates from aqueous EtOH or C6H6-light petroleum, 145° [2,4- dinitrophenylhydrazone, yellow prisms from HOAc, m. 206° (decomposition)]. VIII is dehydrated by warm HOAc and HCl in 30 min. to 2-carbethoxyisoflavone, 92, rectangular plates, 96-7°, which, heated with concentrated H2SO4 30 min. at 100°, then poured into H2O, gives isoflavone-2-carboxylic acid (IX), 73, needles from CHCl3-light petroleum 212-13°. Heating 0.38 g. IX at 220° until gas evolution ceased, crystallizing the product from aqueous EtOH, washing with NaHCO3, and drying gives 0.22 g. isoflavone, m. 131° (from light petroleum), also prepared in 82% yield by the formylation method (Joshi and Venkataraman, C.A. 28, 4421.1) 2,4-HO(MeO)C6H3COCH2Ph (X) is best prepared by the method of Bentley and Robinson (C.A. 45, 151a), but it can readily be prepared by the partial methylation of 2,4-(HO)2C6H3COCH2Ph (XI), m. 110-11° (from C6H6). XI, Me2SO4, K2CO3, and C6H6 boiled 90 min., cooled, filtered, and evaporated give X, 51, needles, 88°. I and X in C5H5N give an oil, possibly 2-carbethoxy-2-hydroxy-7-methoxyisoflavanone, which, warmed with HOAc and concentrated HCl, then added to H2O and crystallized from EtOH, gives 2-carbethoxy-7-methoxyisoflavone (XII), 80, prisms, 130-1°, also prepared (48%) by methylation of 2-carbethoxy-7-hydroxyisoflavone, and (10%) by treating X with Na and (CO2Et)2 then with HOAc. Saponification of XII yields, after acidifying, 7-methoxyisoflavone-2-carboxylic acid, 97, needles from aqueous EtOH, 243° (decomposition), decarboxylated to 7-methoxy-isoflavone, 90, plates from MeOH, 156°. I added to 2,4,6-HO(MeO)2C6H2COCH2Ph (XIII) in C5H5N gives 2-carbethoxy-2-hydroxy-5,7-dimethoxyisoflavanone (XIV), 69, prisms, 148-53°. XIV heated with HOAc and HCl 15 min. at 100° gives 2-carbethoxy-5,7-dimethoxyisoflavone (XV), 85, pale yellow prisms, 156-8°, which, shaken 40 min. with KOH, acidified, dissolved in NaHCO3, filtered, and reacidified, gives 5,7-dimethoxyisoflavone-2- carboxylic acid (XVI), 68, 224° (decomposition). XV, m. 159°, is also prepared (91%) by methylation of 2-carbethoxy-5,7-dihydroxyisoflavone. I, XIII, C5H5N, and C6H6 heated 2.5 hrs. at 100° give an oil which, crystallized from EtOH, yields 2-carbethoxy-2-ethoxalyloxy-5,7- dimethoxyisoflavanone (XVII), 30, needles, 111-12°. XVII in C5H5N shaken with powdered KOH 20 min. and poured into H2O gives 20% XIV (crystallized from H2O). Dehydration of XIV gives XV, also formed by heating XVII 4.5 hrs. with Ac2O and NaOAc. XIII (3 g.), 40 ml. HCO2Et, and 3 g. powdered Na stirred 2 hrs. at -10°, kept 48 hrs. at 0°, and treated with ice and Et2O give 1.9 g. 2-hydroxy-5,7-dimethoxyisoflavanone, prisms from aqueous EtOH, m. 152°, which, warmed with HOAc 30 min. at 100°, gives 5,7-dimethoxyisoflavone (XVIII), prisms from EtOAc, m. 107°, also formed by heating XVI 1-2 min. at 230°. I (5 g.) added to 5 g. of o-HOC6H4COMe in C5H5N and treated with dilute HCl after 15 min. yields an oil which, extracted (CHCl3) and crystallized from light petroleum, gives 5.2 g. o-ethoxalyloxyacetophenone, needles, m. 41°. This undergoes hydrolysis on

storage. Basic reagents do not convert it into a β-diketone. The ultraviolet absorption spectra of genistein and some genistein mono-Me ethers are [compound, λmin. (log ε), λmaximum (log ε), λinflection (log ε); λ given in mμ]: genistein, 231 (4.04), 263 (4.50), 325 (3.71); 7-methyl ether (prunetin), 231 (4.07), 262.5 (4.57), 325 (3.65); 4'-Me ether (biochanin-A), 231 (4.10), 262.5 (4.56), 325 (3.71); 5-Me ether, 227 (4.13), 256 (4.51), 312 (3.81).

IT 15485-80-0P, Isoflavone, 7-hydroxy-4'-nitro-
RL: PREP (Preparation)
(preparation of)

RN 15485-80-0 CAPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-nitrophenyl)- (CA INDEX NAME)



L24 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1953:61964 CAPLUS Full-text

DOCUMENT NUMBER: 47:61964

ORIGINAL REFERENCE NO.: 47:10530e-g

TITLE: Isoflavones. I. Some nitroisoflavones

AUTHOR(S): Dutta, N. L.; Bose, J. L.

CORPORATE SOURCE: Natl. Chem. Lab., Poona

SOURCE: Journal of Scientific & Industrial Research (1952), 11B, 413-15
CODEN: JSIRAC; ISSN: 0022-4456

DOCUMENT TYPE: Journal

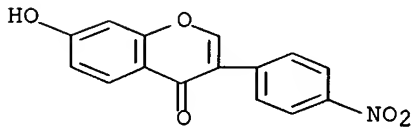
LANGUAGE: Unavailable

AB cf. C.A. 46, 1542d. 2,4-(HO)2C6H3COC6H4NO2-p (I), m. 204°, was prepared in 65% yield from resorcinol and p-O2NC6H4CH2CN by the Hoesch reaction with anhydrous AlCl3 as the condensing agent. I (1 g.), 1 ml. HC(OEt)3, and 5 drops piperidine in dry 12 ml. pyridine were refluxed 7 hrs. at 120°, cooled, filtered, and the precipitate recrystd. to yield 0.7 g. of 7-hydroxy-4'-nitroisoflavone (II), m. 290°; 7-acetate, m. 225° (from alc.); 7-methoxy-4'-nitroisoflavone, m. 245°. I (0.73 g.) refluxed 20 hrs. with 0.8 g. AcONa and 5 ml. Ac2O, and the product recrystd. from EtOH, AcOEt, and Me2CO yielded 0.7 g. of 2-methyl-7-acetoxy-4'-nitroisoflavone (III), m. 245°. Acetylation of I 3 hrs. at 100° gave III in quant. yield. H2SO4 (2.5 ml.) was added to 0.4 g. III at 0° and the mixture stirred and allowed to come to room temperature; addition of ice precipitated 2-methyl-7-hydroxy-4'-nitroisoflavone (IV), m. 310° (from alc.), 2,4,6-Trihydroxyphenyl-p-nitrobenzyl ketone (V), m. 245°. was prepared from phloroglucinol and p-O2NC6H4CH2CN. The 5,7-dihydroxy-, m. 296°, 5,7-diacetoxy-, m. 212°, 2-methyl-5,7-diacetoxy-, m. 190°, and 2-methyl-5,7-dihydroxy-4'-nitroisoflavone, m. 260°, were prepared from V.

IT 15485-80-0P, Isoflavone, 7-hydroxy-4'-nitro-
RL: PREP (Preparation)
(preparation of)

RN 15485-80-0 CAPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-nitrophenyl)- (CA INDEX NAME)

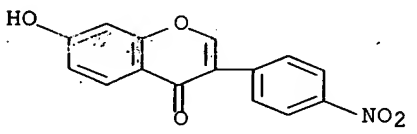


L24 ANSWER 19 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1952:8596 CAPLUS Full-text
DOCUMENT NUMBER: 46:8596
ORIGINAL REFERENCE NO.: 46:1542d-e
TITLE: Synthesis of some nitroisoflavones
AUTHOR(S): Dutta, N. L.; Bose, J. L.
CORPORATE SOURCE: Natl. Chem. Lab., Poona
SOURCE: Journal of Scientific & Industrial Research (1951), 10B, 75
CODEN: JSIRAC; ISSN: 0022-4456
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB 7-Hydroxy-4'-nitroisoflavone (I), m. 290° (from alc.), was obtained in 70% yield by condensing 2,4-dihydroxyphenyl 4'-nitrobenzyl ketone with HC(OEt)3 in pyridine. 2,4,6-Trihydroxyphenyl 4'-nitrobenzyl ketone (II), m. 245° (from alc.), m. 245°, was obtained, in 80% yield by condensing p-O2NC6H4CH2CN with phloroglucinol; with H(COEt)3, it yielded 5,7-dihydroxy-4'-nitroisoflavone, m. 296° (from alc.).

IT 15485-80-0P, Isoflavone, 7-hydroxy-4'-nitro-
RL: PREP (Preparation)
(preparation of)

RN 15485-80-0 CAPLUS
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-nitrophenyl)- (CA INDEX NAME)



L24 ANSWER 20 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1952:8595 CAPLUS Full-text
DOCUMENT NUMBER: 46:8595
ORIGINAL REFERENCE NO.: 46:1541h-i,1542a-d
TITLE: Synthetic experiments in the benzopyrone series. XIII. Constitution of prunetin and its synthesis
AUTHOR(S): Narasimhachari, N.; Seshadri, T. R.
CORPORATE SOURCE: Delhi Univ., India
SOURCE: Proceedings - Indian Academy of Sciences, Section A (1950), 32A, 256-63
CODEN: PISAA7; ISSN: 0370-0089
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

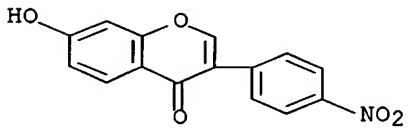
AB cf. C.A. 45, 4714i. Prunetin (I) (C.A. 44, 3988e) was completely ethylated and the constitution of the di-Et ether (7-methoxy-4',5- diethoxyflavone) (II) was established by condensing phloroglucinol (III) with p-EtOC6H4CH2CN (IV), converting the resulting ketone (2,4,6-trihydroxyphenyl p-ethoxybenzyl ketone) (V) into 5,7-dihydroxy-4'-ethoxyisoflavone (VI), partially methylating VI with

1 mole Me2SO4 to 5-hydroxy-7-methoxy-4'-ethoxyisoflavone (VII), followed by complete ethylation with EtI to II. III (5 g.), 5 g. IV, and 1 g. ZnCl2 in 100 ml. Et2O were cooled, saturated 4 hrs. with dry HCl, refrigerated overnight, the Et2O decanted, and the ketimine-HCl dissolved in H2O and heated 1 hr. at 100°, giving V m. 208-10°, on cooling. Treating 1 g. powdered Na with 2 g. V in 10 ml. cold HCO2Et, refrigerating 48 hrs., removing the HCO2Et in vacuo, and extracting with Et2O gave 0.5 g. VI, m. 238-40°, soluble in aqueous Na2CO3, and giving a pink color with FeCl3. Methylating 0.5 g. VI with 0.2 ml. Me2SO4 and 0.5 g. K2CO3 6 hrs. in Me2CO yielded VII, m. 142-4°, giving a deep red color with FeCl3, and sparingly soluble in aqueous NaOH. Refluxing VII in Me2CO 20 hrs. with excess EtI and K2CO3 gave II, m. 116-17°, insol. in aqueous alkali, giving no color with FeCl3. Natural I ethylated like VII gave a product identical with II (mixed m.p.). A simplified synthesis of I by partial methylation of genistein (IX) was possible. IX was prepared by demethylation of I and by the following synthesis: III was condensed with p-MeOC6H4CH2CN and the resulting ketone partially methylated with 2 moles Me2SO4 to 2-hydroxy-4,6-dimethoxyphenyl p-methoxybenzyl ketone (X), which was converted into 4',5,7-trimethoxyisoflavone (genistein tri-Me ether) (XI). Demethylation of XI gave genistein in good yield. Refluxing 4 g. of 2,4,6-trihydroxyphenyl p-methoxybenzyl ketone in Me2CO with 3 ml. Me2SO4 and 6 g. K2CO3 10 hrs., removing the solvent, treating with H2O, extracting with Et2O, extracting the Et2O solution with NaOH, cooling the alkaline extract, and acidifying gave X, m. 88-9°. From X, 1.2 g. XI was obtained like VI. Partial methylation of IX gave I. Refluxing 1 g. IX 4 hrs. in 100 ml. Me2CO with 0.3 ml. Me2SO4 and 1 g. K2CO3, removing the Me2CO, treating with H2O, filtering, and acidifying yielded 0.2 g. I, m. 238-40°, giving a violet color with FeCl3, soluble in NaOH. Acidification of the carbonate solution gave IX. The I acetate prepared from synthetic I was identical with that prepared from natural I (m. and mixed m.p. 224-6°). The di-Et ether was identical to II. Treating 1 g. naringenin in 30 ml. Me2CO in the same way I was prepared from IX gave sakuranetin, m. 152-4°(C.A. 44, 1493d).

IT 15485-80-0P, Isoflavone, 7-hydroxy-4'-nitro-
RL: PREP (Preparation)
(preparation of)

RN 15485-80-0 CAPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-nitrophenyl)- (CA INDEX NAME)



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(FILE 'HOME' ENTERED AT 19:23:35 ON 20 OCT 2007)

FILE 'REGISTRY' ENTERED AT 19:23:46 ON 20 OCT 2007

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L2 50 S SSS SAM L1
L3 STRUCTURE UPLOADED
L4 10 S SSS SAM L3

FILE 'STNGUIDE' ENTERED AT 19:27:21 ON 20 OCT 2007

FILE 'REGISTRY' ENTERED AT 19:50:31 ON 20 OCT 2007

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L5              STRUCTURE UPLOADED
L6           10 S SSS SAM L5
L7          289 S SSS L5 FULL
                SAVE L7 TEMP AVER10523964/A

     FILE 'CAPLUS' ENTERED AT 19:54:33 ON 20 OCT 2007
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                SAVE TEMP AVE10523964/A L8
                E US 2005-523964/APPS
L9            1 S E3
                SEL RN

     FILE 'REGISTRY' ENTERED AT 19:56:17 ON 20 OCT 2007
L10         252 S E1-E252
L11          22 S L10 AND L7

     FILE 'CAPLUS' ENTERED AT 19:58:42 ON 20 OCT 2007
L12          11 S L11
L13           7 S L12 AND (AY<2002 OR PY<2002 OR PRY<2002)

     FILE 'REGISTRY' ENTERED AT 20:10:29 ON 20 OCT 2007
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L16          41 S L14 SSS FULL SUB=L7
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     FILE 'CAPLUS' ENTERED AT 20:12:53 ON 20 OCT 2007
L17          36 S L16
L18          23 S L16 AND (AY<2002 OR PY<2002 OR PRY<2002)
L19          23 S L17 AND (AY<2002 OR PY<2002 OR PRY<2002)
L20          23 S L19 AND L7
L21           0 S L19 NOT L7
L22        4602 S L19 OR L7
L23           3 S L19 AND L13
L24          20 S L19 NOT L13
L25          27 S L19 OR L13
L26           4 S L13 NOT L20

=> fil reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                  127.33     407.66

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY    SESSION
CA SUBSCRIBER PRICE                                  -15.60     -21.06

FILE 'REGISTRY' ENTERED AT 20:25:44 ON 20 OCT 2007
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provided by InfoChem.

STRUCTURE FILE UPDATES:   19 OCT 2007  HIGHEST RN 951118-42-6
DICTIONARY FILE UPDATES:  19 OCT 2007  HIGHEST RN 951118-42-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.
```

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

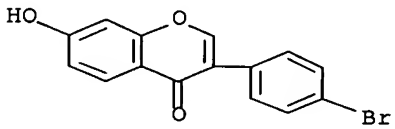
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

```
=> s  (15485-80-0/rn or 96644-05-2/rn)
             1 15485-80-0/RN
             1 96644-05-2/RN
L27          2 (15485-80-0/RN OR 96644-05-2/RN)

=> d scan

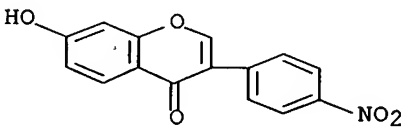
L27  2 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
IN   4H-1-Benzopyran-4-one, 3-(4-bromophenyl)-7-hydroxy- (9CI)
MF   C15 H9 Br O3
```




```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L27  2 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
IN   4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-nitrophenyl)-
MF   C15 H9 N O5
```




```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

ALL ANSWERS HAVE BEEN SCANNED

=> fil reg
COST IN U.S. DOLLARS                    SINCE FILE      TOTAL
                                          ENTRY    SESSION
```

```
FULL ESTIMATED COST                                    1.35      409.01

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)        SINCE FILE      TOTAL
                                                     ENTRY     SESSION
CA SUBSCRIBER PRICE                                   0.00      -21.06

FILE 'REGISTRY' ENTERED AT 20:27:34 ON 20 OCT 2007
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STRUCTURE FILE UPDATES:   19 OCT 2007  HIGHEST RN 951118-42-6
DICTIONARY FILE UPDATES:  19 OCT 2007  HIGHEST RN 951118-42-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> d his

     (FILE 'HOME' ENTERED AT 19:23:35 ON 20 OCT 2007)

     FILE 'REGISTRY' ENTERED AT 19:23:46 ON 20 OCT 2007
L1             STRUCTURE UPLOADED
L2          50 S SSS SAM L1
L3             STRUCTURE UPLOADED
L4          10 S SSS SAM L3

     FILE 'STNGUIDE' ENTERED AT 19:27:21 ON 20 OCT 2007

     FILE 'REGISTRY' ENTERED AT 19:50:31 ON 20 OCT 2007
L5             STRUCTURE UPLOADED
L6          10 S SSS SAM L5
L7         289 S SSS L5 FULL
               SAVE L7 TEMP AVER10523964/A

     FILE 'CAPLUS' ENTERED AT 19:54:33 ON 20 OCT 2007
L8        4602 S L7
               SAVE TEMP AVE10523964/A L8
               E US 2005-523964/APPS
L9           1 S E3
               SEL RN

     FILE 'REGISTRY' ENTERED AT 19:56:17 ON 20 OCT 2007
L10         252 S E1-E252
L11          22 S L10 AND L7
```

```
     FILE 'CAPLUS' ENTERED AT 19:58:42 ON 20 OCT 2007
L12           11 S L11
L13            7 S L12 AND (AY<2002 OR PY<2002 OR PRY<2002)

     FILE 'REGISTRY' ENTERED AT 20:10:29 ON 20 OCT 2007
L14              STRUCTURE UPLOADED
L15            4 S L14 SSS SAM SUB=L7
L16           41 S L14 SSS FULL SUB=L7
                 SAVE TEMP L16 AV10523964/A

     FILE 'CAPLUS' ENTERED AT 20:12:53 ON 20 OCT 2007
L17           36 S L16
L18           23 S L16 AND (AY<2002 OR PY<2002 OR PRY<2002)
L19           23 S L17 AND (AY<2002 OR PY<2002 OR PRY<2002)
L20           23 S L19 AND L7
L21            0 S L19 NOT L7
L22         4602 S L19 OR L7
L23            3 S L19 AND L13
L24           20 S L19 NOT L13
L25           27 S L19 OR L13
L26            4 S L13 NOT L20

     FILE 'REGISTRY' ENTERED AT 20:25:44 ON 20 OCT 2007
L27            2 S  (15485-80-0/RN OR 96644-05-2/RN)

     FILE 'REGISTRY' ENTERED AT 20:27:34 ON 20 OCT 2007

=> s l16 not l27
L28           40 L16 NOT L27

=> save temp l28 walk10523964/a
ANSWER SET L28 HAS BEEN SAVED AS 'WALK10523964/A'

=> logoff h
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY     SESSION
FULL ESTIMATED COST                                    2.25      411.26

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY     SESSION
CA SUBSCRIBER PRICE                                    0.00      -21.06

 SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 20:30:29 ON 20 OCT 2007
```